Pomeranchuk cooling of the SU($2N$) ultra-cold fermions in optical lattices

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We investigate the thermodynamic properties of a half-filled SU($2N$) Fermi-Hubbard model in the two-dimensional square lattice using the determinantal quantum Monte Carlo simulation, which is free of the fermion "sign problem". The large number of hyperfine-spin components enhances spin fluctuations, which facilitates the Pomeranchuk cooling to temperatures comparable to the superexchange energy scale at the case of SU(6). Various quantities including entropy, charge fluctuation, and spin correlations have been calculated.

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The SU($2N$) and Sp($2N$) Fermi-Hubbard and Heisenberg models were originally introduced to condensed matter physics as a mathematic convenience [1–4]. They generalize the SU(2) models of electrons and enable the $1/N$-expansion to systematically handle strong correlations. In the cold atom context, it was proved that the large spin Fermi systems with the hyperfine spin $F=\frac{3}{2}$ possess a generic Sp(4), or, isomorphically SO(5) symmetry, without fine tuning [5, 6]. It can be augmented to the even higher symmetry of SU(4) with alkaline-earth fermions due to their fully filled electron shells [5]. In this case, their hyperfine spins completely come from nuclear spins, thus interactions are spin-independent. The recent development of ultra-cold Fermi gases has provided an opportunity to realize these high symmetries, thus they are not just of academic interests. Experimentally, the SU(6) symmetric system of ^{173}Yb with $F=I=\frac{5}{2}$ and the SU(10) symmetric one of ^{87}Sr with $F=I=\frac{9}{2}$ have been cooled down to quantum degeneracy [7–9]. The study of SU($2N$) by using alklaine-earth fermions was also proposed in Ref. [10].

The properties of large spin ultra-cold Fermi gases with SU($2N$) and Sp($2N$) symmetries are fundamentally different from those of large spin solid state systems [11]. In the former case, quantum spin fluctuations are enhanced by the large number of fermion components denoted by $2N=2F+1$, which are even stronger than those in spin-$\frac{1}{2}$ systems. On the contrary, the large value of spin suppresses quantum fluctuations in solid state systems, and drives the system to the classic limit. The novel physics in large-spin ultra-cold Fermi systems with high symmetries includes unconventional superfluidity [12–16], exotic quantum magnetism [17–21]. In particular, various SU($2N$) valence-bond solid and spin liquids have been proposed that have not been observed in solid state systems [22–24].

In current experiments, ultracold fermions in optical lattices have been cooled down to temperatures below the hopping energy scale of t, but, above the spin superexchange energy scale of J yet. This motivates us to study the thermodynamic properties of the ultracold fermions in this temperature regime. On the other hand, the strong correlation physics of the Fermi-Hubbard model in this intermediate temperature regime is also interesting, which has not been fully explored yet in solid state physics context. In cuprates, J is around 1000K at which lattices melt. In this temperature regime, the intertwined effect between the quantum and thermodynamic fluctuations leads to interesting phenomena. The quantum critical phenomena have been studied in the SU(2) case [25, 26]. Recently, the high temperature properties of SU($2N$) Hubbard model has been studied from series expansions, which is only accurate at $T \gg \max(t,U)$ [27].

In this paper, we focus on the intermediate temperature regime ($t > T \sim J$) of current experiment interests and study the thermodynamic properties of the half-filled SU($2N$) Fermi-Hubbard model in 2D square lattice using the determinantal Quantum Monte Carlo (DQMC) simulation [28, 29], which is an unbiased, non-perturbative method. It is free of the sign problem at half-filling, which enable us to obtain reliable results down to low temperatures ($T/t \sim 0.1$). Various thermodynamic quantities are calculated for different values of $2N$. Special attentions are devoted to the interaction-induced adiabatic cooling, that the system is cooled down to the temperature scale around J by adiabatically increasing interactions. This Pomeranchuk cooling effect, though it is very weak in the SU(2) case [30, 31], appears in the SU(6) case, which can cool the system to temperature lower than J. This is relevant to the experiment systems of ^{173}Yb.

We consider the following SU($2N$) Fermi-Hubbard model defined in the 2D square lattice at half-filling as

$$H=-t\sum_{\langle i,j\rangle,\alpha}\left(c^{\dagger}_{i\alpha}c_{j\alpha}+h.c.\right)+\frac{U}{2}\sum_{i}\left(n_i-N\right)^2, \quad (1)$$

where α runs over the $2N$ components; $\langle i,j\rangle$ denotes the summation over the nearest neighbors; n_i is the to-

tal particle number operator on site i defined as $n_i = \sum_{\alpha=1}^{2N} c_{i\alpha}^\dagger c_{i\alpha}$. Eq.(1) is invariant under the particle-hole transformation in bipartite lattices. Similarly to the case of SU(2), it is easy to prove that the sign problem is also absent for the half-filled SU($2N$) Hubbard model of Eq. 1 in bipartite lattices in the DQMC simulations.

Below we will present our DQMC simulations for thermodynamic quantities for the SU($2N$) Hubbard model with $2N = 4$ and 6 in the square lattice of $L \times L$ with the periodical boundary condition. The second order Suzuki-Trotter decomposition is used. The Trotter steps are taken $\Delta\tau = \beta/M$ where $\beta = 1/T$ is the inverse of the temperature T and M ranges from 30 to 100 depending on temperatures. We have checked that the convergence of the simulation results with respect to different values of $\Delta\tau$. Instead of using the Hubbard-Stratonovich (HS) transformation in the spin channel [32], we adopt the HS transformation in the charge channel which maintains the $SU(2N)$ symmetry explicitly [33]. This method gives rise to errors of the order of $(\Delta\tau)^4$.

We will first address the possibility of cooling down the system by adiabatically increasing the repulsive interaction. For spinful fermion systems (e.g. ^{3}He), the Pomeranchuk effect refers to the fact that increasing temperatures can lead to solidification because the entropy (per particle) in the localized solid phase is larger than that of the itinerant Fermi liquid phase. The reason is that in the Fermi liquid phase, only fermions close to Fermi surface within T contribute to entropy, while in solids each site contributes to nearly $\ln 2 \approx 0.69$ if T is comparable to the spin exchange energy scale of J, which is much smaller than the Fermi energy. $J/t \approx 4t/U$ in the strong coupling regime, and $J/t \propto e^{-2\pi\sqrt{\frac{t}{U}}}$ in the weak coupling regime. It reaches maximum in the intermediate coupling regime. In the lattice systems near or at half-filling, increasing interaction suppresses charge fluctuations and drives systems to the Mott-insulating state, thus we would expect Pomeranchuk cooling during adiabatically increasing interactions[34]. However, for the SU(2) Hubbard model, both at 2D and 3D, DQMC simulations show that the effect of Pomeranchuk cooling is not obvious at half-filling [30, 31, 35]. This is because for the SU(2) case, the tendency towards magnetic ordering is strong at temperatures lower than J, which suppresses the entropy capability in the Mott insulating state [30].

In Fig. 1, curves of the simulated entropy per particle (not per site) $S_{su(2N)}$ *v.s.* $2N$, are plotted. $S_{su(2N)}$ is defined as $S_{su(2N)} = S/(NL^2)$, where S is the total entropy in the lattice. It is calculated from the formula

$$\frac{S_{su(2N)}(T)}{k_B} = \ln 4 + \frac{E(T)}{T} - \int_T^\infty dT' \frac{E(T')}{T'^2}, \qquad (2)$$

where $\ln 4 \approx 1.38$ is the entropy at the infinite temperature, or, equivalently, $T \gg U$; $E(T)$ denotes the average internal energy per particle at temperature T. The interaction parameters are chosen for the free case ($U/t = 0$),

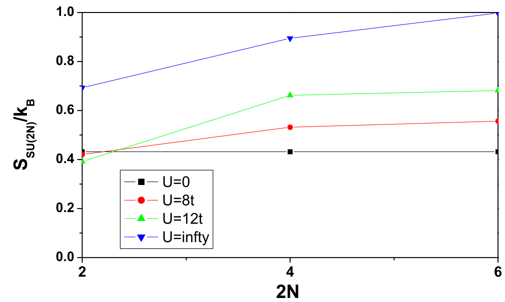

FIG. 1: Entropy per particle $S_{su(2N)}$ for the SU($2N$) Hubbard model at half-filling v.s. $2N$ in a 10×10 square lattice. The temperature is fixed at $T/t = \frac{1}{3}$. The line of $U/t = \infty$ is from the results of Eq. 3.

the intermediate ($U/t = 8$) and strong ($U/t = 12$) interaction strengths, and also the limit of $U/t = \infty$. The temperature $T/t = \frac{1}{3}$ is low compared to the band width $W/t = 8$, and is comparable to J for $U/t = 8$ and 12 around which spin exchange is strongest. The results of the SU(2) case are consistent with those in Ref. [30]. At $U/t = 8$ and 12, $S_{su(2)}$ becomes even smaller than that at $U/t = 0$, which shows effectiveness of suppressing entropy from spin correlations. Consequentially, we do not expect the Pomeranchuk cooling in this interaction regime. If further increasing U/t to very large values, finally J will become much smaller than T, and in this case we expect that $S_{su(2)}/k_B$ will grow and saturate at the $\ln 2$ at $U/t \to \infty$. This situation changes at the cases of SU(4) and SU(6) at half-filling. The entropies per particle at intermediate and strong interaction strengths are larger than that of the free case which is independent of $2N$. This means that for the cases of SU(4) and SU(6) with a larger number of fermion components, the temperature scale comparable to J is already sufficient to suppress spin correlations. For $U/t = \infty$, J is suppressed to zero, and thus T/J is set to infinity, $S_{su(2N)}$ can be calculated analytically as

$$\frac{S_{su(2N)}}{k_B} = \frac{1}{N} \ln \frac{(2N)!}{(N!)^2}, \qquad (3)$$

which grows monotonically as increasing $2N$ and saturates at $\ln 4$ as $2N \to \infty$.

The above picture gives rise to the main point of this work: the Pomeranchuk effect in SU($2N$) Fermi-Hubbard model becomes observable at intermediate interaction strengths starting from the cases of SU(4) and SU(6). This is because the magnetic correlations are weakened by the large-N effect. We have confirmed this picture by performing DQMC simulations for various parameter values of T and U for the SU(6) case, which is of direct relevancy to the current experimental interests about ultracold ^{173}Yb atoms[7]. The isoentropy curves

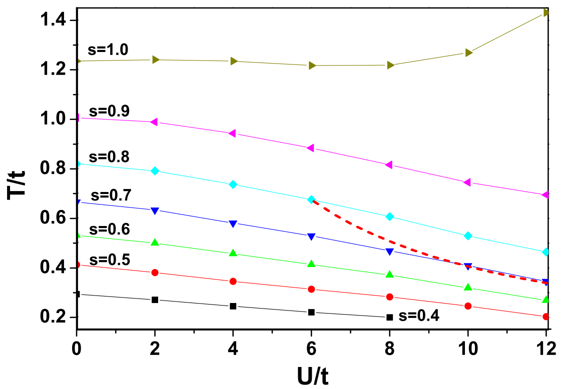

FIG. 2: The isoentropy curves for the half-filled SU(6) Hubbard model in a 10×10 square lattice. The dashed line denotes the spin superexchange scale in strong coupling regime $J/t = 4t/U$

are displayed in Fig.2. For low values of the entropy, say, $S_{su(6)}/k_B < 0.7$, adiabatic increasing U leads to a significant cooling to a temperature below the magnetic superexchange scale J, which means that in this case, the Pomeranchuk cooling can overwhelm the decreasing of J when we adiabatically increasing U, thus finally cool the system to the spin superexchange temperature regime. Different from Ref. [27], we fix filling factor instead of total particle number, thus the entropy in the non-interacting case does not scale as $N^{\frac{1}{3}}$ as they presented, but also scales linearly with N as the same as those in the half-filled Mott-insulating states.

Next we study the simulations of charge fluctuations for the half-filled SU($2N$) Hubbard model. The normalized on-site charge fluctuations are defined as

$$\delta_{su(2N)} = \sqrt{\frac{\langle n_i^2\rangle - \langle n_i\rangle^2}{N}}, \tag{4}$$

where $\langle n_i\rangle = N$. At $T \to \infty$, $\delta_{su(2N)}$ can be calculated exactly which is independent of $2N$ as $\delta_{su(2N)}(T\to\infty) = \frac{\sqrt{2}}{2} \approx 0.71$, which is the upper limit. Similarly, at $U = 0$, $\delta_{su(2N)}$ is the same as $\frac{\sqrt{2}}{2}$ and is independent on both $2N$ and T. For the general case, we plot the DQMC simulation results of δ at a relatively weak interaction $U/t = 4$ for a large range of temperatures in Fig. 3 (a). For all the cases, $\delta_{su(2N)}$ is suppressed by U from the upper limit of $\frac{\sqrt{2}}{2}$ due to interaction. For the cases of SU(4) and SU(6), $\delta_{su(2N)}(T)$ first falls as T increases, which is a reminiscence of the Pomeranchuk effect. After reaching a minimum at T comparable to t, $\delta_{su(2N)}$ grows as increasing T. This indicates that fermions are the most localized at an intermediate temperature scale at which the spin channel contribution to entropy dominates. For

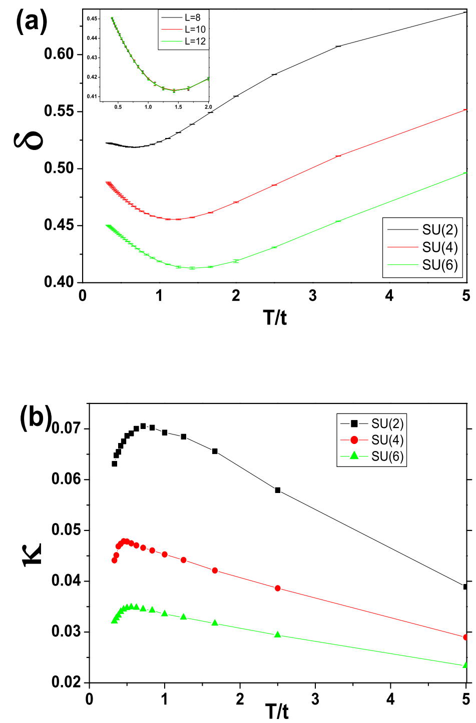

FIG. 3: a) The on-site charge fluctuations δ as a function of temperature T with parameters $U/t = 4$ and different values of $2N$ for a 10×10 lattice. The inset shows the convergence of $\delta(T)$ with $L = 8, 10$, and 12 for the SU(6) case. b) The normalized compressibility $\kappa_{su(2N)}/(2N)$ v.s. T at $U/t = 4$.

the SU(2) case, the non-monotonic behavior of $\delta_{su(2N)}$ is not obvious. This agrees with the picture that large values of $2N$ enhances spin fluctuations, and enhances the Pomeranchuk effect.

The physical observable compressibility κ can be expressed in terms of the global charge fluctuations as

$$\kappa_{su(2N)} = \frac{1}{L^2}\frac{\partial N_f}{\partial \mu} = \frac{1}{TL^2}(\langle \hat{N}_f^2\rangle - \langle \hat{N}_f\rangle^2), \tag{5}$$

where $\hat{N}_f = \sum_i \hat{n}_i$ is the total fermion number operator in the lattice; μ is the chemical potential. In Fig. 4 (b), we plot the simulated results for the normalized $\kappa_{su(2N)}/N$, i.e., the contribution to $\kappa_{su(2N)}$ per fermion component. They behave similarly with each other. $\kappa_{su(2N)}$ scales as $1/T$ like ideal gas at high temperatures, while they are suppressed at low temperatures. At zero temperature, $\kappa_{su(2N)}$ is suppressed to zero due to the charge gap in the Mott-insulating states. $\kappa_{su(2N)}$ reaches the maximum at an intermediate temperature scale which can be attributed to the charge fluctuation energy scale.

Next we study spin correlations of the SU($2N$) Hubbard model. The SU($2N$) generators can represented through fermion operators $c_{i,\alpha}(\alpha = 1 \sim 2N)$ as $M_{\alpha\beta,i} =$

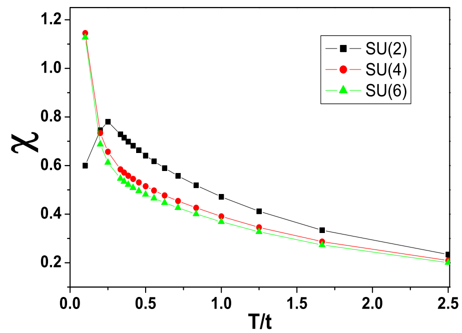

FIG. 4: The normalized SU($2N$) susceptibilities $\chi_{su(2N)}$ v.s. T with fixed $U/t = 4$ for $2N = 2, 4, 6$

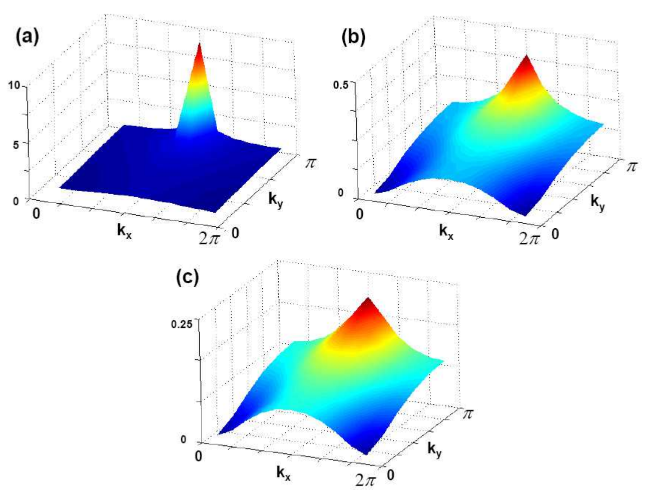

FIG. 5: The normalized spin structure factor $S(\vec{q})$ for half-filled SU($2N$) Hubbard model for $2N$ equal to (a) 2, (b) 4, and (c) 6. Parameter values are $T/t = 0.1$, and $U/t = 8$.

$c^\dagger_{\alpha,i} c_{\beta,i} - \frac{1}{2N}\delta_{\alpha\beta} n_i$. There are only $(2N)^2 - 1$ independent operators due to the constraint $\sum_\alpha M_{\alpha\alpha} = 0$. They satisfy the commutation relations as $[M_{\alpha\beta,i}, M_{\gamma\delta,j}] = \delta_{i,j}(M_{\alpha\delta,i}\delta_{\gamma\beta} - M_{\gamma\beta,i}\delta_{\alpha\delta})$. Due to the Fierz identity, the on-site SU($2N$) fluctuations are related to the onsite particle number $\hat{n}_i = \sum_\alpha c^\dagger_{\alpha,i} c_{\alpha,i}$ as $\sum_{\alpha\beta} M_{\alpha\beta,i} M_{\beta\alpha,i} = \frac{(2N+1)N}{2} - \frac{2N+1}{2N}(\hat{n}_i - N)^2$. We define the SU($2N$) version of two point equal time spin-spin correlation as

$$M_{spin}(i,j) = \frac{1}{(2N)^2 - 1}\langle \sum_{\alpha,\beta} M_{\alpha\beta,i} M_{\beta\alpha,j} \rangle. \qquad (6)$$

At finite temperatures, no magnetic long-range-order should exist in the 2D half-filled SU($2N$) model due to its continuous symmetry of SU($2N$). The normalized uniform SU($2N$) spin susceptibility is defined as

$$\chi_{su(2N)}(T) = \frac{\beta}{NL^2} \sum_{\vec{i},\vec{j}} M_{spin}(i,j). \qquad (7)$$

The DQMC simulation results are presented in Fig. 4 for $U/t = 4$. At high temperatures, $\chi_{su(2N)}$ exhibits the standard Curie-Weiss law which scales proportional to $1/T$. $\chi_{su(2N)}$ reaches the maximum at an intermediate temperature at the scale of J below which $\chi_{su(2N)}$ is suppressed by the AF exchange. The nature of the ground states of half-filled $SU(2N)$ Hubbard model remains an open question in literatures when $2N$ is small but larger than 2. Nevertheless, we expect that they either AF long-range-ordered like the case of $SU(2)$, or quantum paramagnetic with or without spin gap like in the large-N limit. In either case, $\chi_{su(2N)}$ is suppressed to zero approaching zero temperature. The spin structure factors $S_{su(2N)}(\vec{q})$ are calculated at half-filling and a low temperature, which are defined as

$$S_{su(2N)}(\vec{q}) = \frac{1}{NL^2} \sum_{\vec{i},\vec{j}} e^{i\vec{q}\cdot\vec{r}} M_{spin}(i,j), \qquad (8)$$

where $\vec{r}$ is the relative vector between sites i and j. The distributions of $S_{su(2N)}(\vec{q})$ with $2N = 2, 4, 6$ are plotted in Fig. 5 a), b) and c) respectively. The sharpness of the peaks at $\mathbf{q} = (\pi, \pi)$ indicates the dominant AF correlations in all the cases. As increasing $2N$, peaks are broadened showing the weakening of the AF correlations.

We have used the DQMC method to simulate the thermodynamic properties of the two-dimensional SU($2N$) fermion Hubbard model at half-filling in the temperature regime of direct interest of current experiments. The large numbers of fermion components enhance spin fluctuations, which facilitates the Pomeranchuk cooling to temperatures comparable to the superexchange energy scale. The local charge fluctuation, compressibility, spin-susceptibility, and spin structural factor are also investigated.

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